

(2-Chloroethylthiopropyl) (2-allylthioethyl) ether

Inchi:	InChI=1S/C10H19ClOS2/c1-2-7-13-10-6-12-5-3-8-14-9-4-11/h2H,1,3-10H2
InchiKey:	ZIEGNUPVQYZNGX-UHFFFAOYSA-N
Formula:	C10H19ClOS2
SMILES:	C=CCSCCOCCSCCCI
Mol. weight [g/mol]:	254.84

Physical Properties

Property code	Value	Unit	Source
gf	70.47	kJ/mol	Joback Method
hf	-188.52	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	57.61	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	3.284		Crippen Method
mcvol	198.270	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinsol	1958.00		NIST Webbook
tb	622.29	K	Joback Method
tc	828.32	K	Joback Method
tf	321.65	K	Joback Method
vc	0.751	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.15	J/mol×K	622.29	Joback Method
cpg	483.57	J/mol×K	656.63	Joback Method
cpg	497.23	J/mol×K	690.97	Joback Method
cpg	510.13	J/mol×K	725.30	Joback Method
cpg	522.27	J/mol×K	759.64	Joback Method
cpg	533.67	J/mol×K	793.98	Joback Method
cpg	544.32	J/mol×K	828.32	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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